## Biophysical Chemistry 6582 <br> Exam 1 <br> MARCH 1, 2004,

I will not cheat today, signed $\qquad$ print name: K_ KEY

1. (25) Consider a two-dimensional unit cell with a axis $=100$ and b axis $=100$, with gamma $=90$,
(a) sketch the cell, and add the 32 planes,
(b) in (a) illustrate Braggs law, sketch two incoming and outgoing rays, indicate the angle theta, the d-spacing and the path difference,

(no calculations are required to answer c-h, circle the correct response)
(c) would the d-spacing for the 33 planes be
less than, greater than, or equal to
the d-spacing for the 44 planes? [comment: increasing $\mathbf{h}$ and $\mathbf{k}$ decreases the spacing]
(d) would the d-spacing for the 33 planes be
less than, greater than, or equal to
the d-spacing for the 23 planes? [decreasing either $\mathbf{h}$ or $\mathbf{k}$ alone increases the spacing]
(e) would the d-spacing for the 33 planes be
less than, greater than, or equal to
the d-spacing for the 32 planes?
(f) would the angle theta for the 33 planes be
less than, greater than, or equal to the angle theta for the 44 planes? [increasing the d spacing decreases $\theta(\mathbf{n} \lambda=\mathbf{2 d} \sin \theta)$ ]
(g) would the angle theta for the 33 planes be
less than, greater than, or equal to
the angle theta for the 23 planes?
(h) would the angle theta for the 33 planes be less than, greater than, or equal to the angle theta for the 32 planes?
2) (25) Indicate the point symmetry (not necessarily the point group) of the following molecules (draw the molecule and the symmetry operators:
a) Water $\left(\mathrm{H}_{2} \mathrm{O}\right)$

A twofold bisects the $\mathrm{H}-\mathrm{O}-\mathrm{H}$ bonds. One mirror is in the plane of the three atoms $\mathrm{H}, \mathrm{O}, \mathrm{H}$. A second mirror is perpendicular to first, and contains the twofold axis.
b) Carbon tetrachloride $\left(\mathrm{CCl}_{4}\right)$

There are threefolds along each $\mathrm{C}-\mathrm{Cl}$ bond. Twofolds bisect each pair of $\mathrm{C}-\mathrm{Cl}$ bonds There are mirrors in the plane of each set of $\mathrm{Cl}-\mathrm{C}-\mathrm{Cl}$.
c) CIFClBr (Carbon bonded with 4 different kinds of halogen atoms)

No symmetry at all.
3) (25) For the questions below:
(For full credit, the c-displacement indicators must be equal to or less than 0 , and equal to or less than 1 )
(a) Sketch a $6_{1}$ screw axis (viewing down the screw axis, i.e., the c -axis) with all the equivalent positions.

(b) Sketch a $6_{4}$ screw axis (viewing down the axis) with all the equivalent positions.

4) (25) Add the equivalent positions to the symmetry elements below.


